

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization International Bureau



(43) International Publication Date
1 September 2005 (01.09.2005)

PCT

(10) International Publication Number
WO 2005/079263 A2

(51) International Patent Classification: Not classified (81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(21) International Application Number: PCT/US2005/004180

(22) International Filing Date: 11 February 2005 (11.02.2005)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data: 60/543,940 13 February 2004 (13.02.2004) US

(71) Applicant (for all designated States except US): WATERS INVESTMENT LIMITED [US/US]; 109 Lukens Drive, New Castle, DE 19720 (US).

(72) Inventors; and

(75) Inventors/Applicants (for US only): GORENSTEIN, Marc. V. [US/US]; 313 Brookline Street, Needham, MA 02492 (US). PLUMB, Robert, S. [US/US]; 6 McGill Lane, Milford, MA 01757 (US). STUMPF, Chris, L.; 28 Highview Drive, Uxbridge, MA 01569 (US).

(74) Agents: GOTTS, Lawrence, J. et al.; Shaw Pittman LLP, 1650 Tysons Boulevard, Mc Lean, VA 22102-4859 (US).

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

— without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

WO 2005/079263 A2

(54) Title: APPARATUS AND METHOD FOR IDENTIFYING PEAKS IN LIQUID CHROMATOGRAPHY/MASS SPECTROMETRY DATA AND FOR FORMING SPECTRA AND CHROMATOGRAMS

(57) Abstract: Chromatograms and mass spectra produced by an LC/MS system are analyzed by creating a two-dimensional data matrix of the spectral and chromatographic data. The two-dimensional matrix can be created by placing the spectra generated by the mass spectrometer portion of the LC/MS system in successive columns of the data matrix. In this way, the rows of the data matrix correspond to chromatographic data and the columns of the data matrix correspond to the spectra. A two-dimensional filter is specified and applied to the data matrix to enhance the ability of the system to detect peaks associated with ions. The two-dimensional filter is specified according to desired criteria. Rank-1 and rank-2 filters can be specified to improve computational efficiency. One method of applying the two-dimensional filter is through convolution of the data matrix with the two-dimensional filter to produce an output data matrix. Peaks corresponding to detected ions are identified in the output data matrix. Parameters of the peaks are determined and stored for later processing including quantitation, or simplification of chromatograms or spectra by, for example, identifying peaks associating with ions having retention times falling within a specified retention time window or having mass-to-charge ratios falling within a specified mass-to-charge ratio window.